Statistical mechanics of thermal contact between system and bath with long-range interactions

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Abstract

In this paper, we address the possibility of generalising the standard analysis of thermal contact between a sample system and a heat bath, by including long range interactions between them. As a concrete example, both system and bath are treated within the long range Ising model. For this model, we derive the equilibrium probability distribution of the energy of the sample system. Equilibrium properties of the system magnetisation and stability of the solutions is discussed. We find existence of a metastable phase below a critical temperature of the bath.

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I. INTRODUCTION

The theory of equilibrium thermodynamics and statistical mechanics has been rigorously developed only for the case of short range interactions among the components of the system. The presence of long range interactions among different components, makes a system much more complex and the standard approaches become inapplicable. Currently, there is a lot of interest to develop new methods and tools to deal with systems involving long range interactions [1]. Apart from the standard examples within the fields of cosmology and astrophysics [2], a growing number of physical laboratory systems have recently emerged in which the interactions are long-ranged, notably in the areas of plasma physics [3], nuclear physics and atomic clusters [4], Bose-Einstein condensates [5], 2D hydrodynamics [6, 7], magnetism [8, 9, 10, 11] and so on (see [1] and references therein). In systems with long range interactions, energy is generally nonadditive. Due to this feature, the thermodynamics of such systems displays unusual properties, like inequivalence of different ensembles [12, 13], possible temperature discontinuity at first order transitions and negative specific heat in microcanonical ensemble [14].

Now the standard derivation of Boltzmann-Gibbs distribution considers a thermal contact between a sample system and a heat bath with a very large heat capacity. The derivation assumes an additive property for energy, to arrive at the desired result. The case of long range interactions between the system and bath seems to be beyond the scope of this derivation [1]. For one, to include such interactions, we have to specify the nature of the interactions between the components of the system and the bath. This implies specifying the microscopic structure of the bath also which makes the characterisation of the bath more detailed. In contrast, within canonical ensemble the bath is characterised only by its temperature irrespective of its microscopic model. Further, nonadditivity of energy brings additional difficulties.

In this paper, we consider this latter case and derive the probability distribution for a system in thermal contact with a heat bath in the presence of long range interactions. In section II, we take a specific model for long range interactions of mean-field type between the system and the bath, and present such a derivation. In section III, we compare our model with the Curie-Weiss model which is paradigmatic model for ferromagnetism. In section IV, equilibrium value of the magnetisation is discussed and stability of the solutions

is highlighted. The last section V, presents a summary of our approach and results.

IIA. Canonical Ensemble from Microcanonical Ensemble

For the sake of completeness and to fix the notation, let us review one of the text-book derivations of the canonical ensemble [15]. Denote by E_1 the energy of the sample and by E_2 the energy of the reservoir. The sample and the reservoir together form an isolated system and the interactions between them are usually considered to be short ranged. Thereby the total energy of the composite system say E_0, is given by the sum of energies $E_1 + E_2$ and is constant. Next, $\Omega_i(E_i)$ where $i = 1, 2$, denote the respective number of microstates at the given values of energies. The probability that the system 1 is in a certain microstate of energy E_1 is given by

$$p_1(E_1) = \frac{\Omega_1(E_1)\, \Omega_2(E_2)}{\Omega_{1+2}(E_0)}, \tag{1}$$

where $E_2 = E_0 - E_1$, and $\Omega_{1+2}(E_0)$ is the total number of states available for the composite system $1 + 2$. Thermodynamic entropy of the reservoir is given by Boltzmann's formula:

$$S_2(E_2) = k_{\rm B} \ln \Omega_2(E_2). \tag{2}$$

Therefore, $p_1(E_1) \propto \Omega_1(E_1)\, e^{S_2/k_{\rm B}}$. In the following, we keep by $k_{\rm B} = 1$ for simplicity. Now expand $S_2(E_2)$ around the most probable value $\bar{E}_2$ as:

$$S_2(E_2) = S_2(\bar{E}_2) + \left(\frac{dS_2}{dE_2}\right)_{\bar{E}_2} (E_2 - \bar{E}_2) + \cdots . \tag{3}$$

As the assumed size of the bath is quite large, its instantaneous energy will be very close to the most probable energy. Therefore, taking $E_2 - \bar{E}_2$ to be small, the higher order terms in the above expansion are negelected. Let the inverse temperature parameter $(dS_2/dE_2)_{\bar{E}_2} = \bar{\beta}_2$. Then using additive property of the energy, we have $E_2 - \bar{E}_2 = \bar{E}_1 - E_1$ and thus we obtain the Boltzmann distribution for system energies: $p(E_1) \propto \Omega_1(E_1)\ \exp(-\bar{\beta}_2 E_1)$.

IIB. ISING MODEL WITH LONG RANGE INTERACTIONS

Now consider the Ising spin model for both the system and the bath interacting with each other through long range interactions. (For a recent discussion of mutual thermal

equilibrium and alternate thermodynamic descriptions within this model, see Ref. [16].)

Take a lattice of N spins with the hamiltonian given by

$$E = -\sum_{j} h_j\ \sigma_j - \sum_{<jk>} \mathcal{J}_{jk}\ \sigma_j\ \sigma_k. \tag{4}$$

Each spin variable σ_i is defined over the set $\{+1, -1\}$. The total system is assumed to be separated into two regions representing a sample system and a heat bath. The spin excess in each region is given by $e_i = N_i^+ - N_i^-$, where $N_i^{\pm}$ are the number of up (+) and down (-) respectively. $\mathcal{J}_{jk}$ and h_j are the known coupling constants within each region which for simplicity, are taken to be constant over a region. We focus on the ferromagnetic interactions which mean $\mathcal{J}$'s are greater than zero. In terms of new variables $E_i = -h_i e_i$, sometimes called the *local energies*, the total energy upto a constant term, can be written in the form

$$E = E_1 + E_2 - a{E_1}^2 - b{E_2}^2 - cE_1 E_2, \tag{5}$$

where a, b and c are suitably defined constants to be elaborated later. Clearly, in the presence of long ranged interactions, the energies as well as the temperatures of the systems, get modified. For example, the most probable energy of system 1 is $\mathcal{E}_1 = \bar{E}_1 - a{\bar{E}_1}^2$ and its inverse temperature is

$$\beta_1^* \equiv \frac{dS_1}{d\mathcal{E}_1} = \frac{\bar{\beta}_1}{(1 - 2a\bar{E}_1)}, \tag{6}$$

where $\bar{\beta}_1 = dS_1/d\bar{E}_1$ is the inverse temperature in the absence of long range interactions within system 1. Similarly, for the bath we have

$$\beta_2^* = \frac{\bar{\beta}_1}{(1 - 2b\bar{E}_2)}. \tag{7}$$

In the following, we adapt the scheme as given in Eqs. (1)-(3) to the case when the total energy is given by (5). It is convenient to express the entropy of a system in terms of the respective local energy E_i. To evaluate $(E_2 - \bar{E}_2)$ for this case, we proceed as follows:

In terms of the most probable values of the local energies, we have

$$E = \bar{E}_1 + \bar{E}_2 - a{\bar{E}_1}^2 - b{\bar{E}_2}^2 - c\bar{E}_1\bar{E}_2. \tag{8}$$

Equating Eqs. (5) and (8) and defining $\Delta E_i = E_i - \bar{E}_i$, $i = 1, 2$, we can write

$$\Delta E_1 + \Delta E_2 - a({E_1}^2 - {\bar{E}_1}^2) - b(E_2 + \bar{E}_2).\Delta E_2 - c(E_1 E_2 - \bar{E}_1 \bar{E}_2) = 0. \tag{9}$$

Now due to the large size of the system 2, the energy E_2 is very closely approximated by its most probable value. Thus the following terms in the above equation can be approximated as

$$(E_2 + \bar{E}_2).\Delta E_2 \simeq 2\bar{E}_2.\Delta E_2, \tag{10}$$

and

$$(E_1 E_2 - \bar{E}_1 \bar{E}_2) \simeq \bar{E}_2.\Delta E_1. \tag{11}$$

Using the above relations in Eq. (9), we get the expression

$$\Delta E_2 = \frac{-\Delta E_1 (1 - c\bar{E}_2) + a({E_1}^2 - {\bar{E}_1}^2)}{(1 - 2b\bar{E}_2)}. \tag{12}$$

Finally, substituting (12) in (3), we arrive at the probability distribution for energies of system 1,

$$p(E_1) = \frac{\Omega_1(E_1)\; e^{-\beta_2^* \{(1 - c\bar{E}_2)E_1 - a{E_1}^2\}}}{\mathcal{Z}}, \tag{13}$$

where

$$\mathcal{Z} = \sum_{E_1} \Omega_1(E_1) \exp\left(-\beta_2^* \{(1 - c\bar{E}_2)E_1 - a{E_1}^2\}\right), \tag{14}$$

the sum being over the range of energies accessible to system 1. It is appropriate here to explain the various paramters above:

$$a = \frac{J_1}{2N_1{h_1}^2}, \quad b = \frac{J_2}{2N_2{h_2}^2}, \quad c = \frac{J_{12}}{N_2 h_1 h_2}. \tag{15}$$

The scaling of parameters by the number of particles is in the same spirit as Kac's priscription [17] and it guarantees that the effective hamiltonian (see Eq. (16) below) is extensive and thus a proper thermodynamic limit is ensured.

III. ANALOGY WITH CURIE-WEISS MODEL

Clearly, when there are no interactions with or within the bath, i.e. $J_2 = J_{12} = 0$ implying $b = c = 0$, then we obtain the probability distribution of the Curie-Weiss model [18] which is described within canonical ensemble with hamiltonain $H = E_1 - a{E_1}^2$ and the bath at inverse temperature $\bar{\beta}_2$.

As mentioned above, the presence of long range interactions within the bath has the effect of modifying the bath temperature to β_2^*. On the other hand, the long range interactions between the system and the bath are incorporated effectively as a modified external magnetic field. This can be clearly seen by noting that the distribution (13) corresponds to an effective hamiltonian $H' = (1 - c\bar{E}_2)E_1 - a{E_1}^2$. In terms of the magnetisation per spin, $y_i = \sum_i \sigma_i/N_i = -E_i/(h_i N_i)$ and using definitions (15) for the parameters, we can write

$$H'(y_1) = -N_1 \left[(h_1 + J_{12}\bar{y}_2)y_1 + \frac{1}{2}J_1{y_1}^2 \right], \tag{16}$$

indicating the extensive property of the effective hamiltonian. Note that the effective applied field is $(h_1 + J_{12}\bar{y}_2) \equiv (1 - c\bar{E}_2)h_1$, where h_1 is the actual applied field. We note that in contrast to the canonical ensemble, in the present case, the bath has a specific microscopic realisation. The expression for the entropy of bath given by Eq. (2), corresponding to the most probable value of magnetisation per spin $\bar{y}_2$ is

$$S_2(\bar{y}_2) = -N_2 \left[\frac{(1+\bar{y}_2)}{2} \ln \frac{(1+\bar{y}_2)}{2} + \frac{(1-\bar{y}_2)}{2} \ln \frac{(1-\bar{y}_2)}{2} \right]. \tag{17}$$

The most probable energy of the bath given by $\mathcal{E}_2 = \bar{E}_2 - b{\bar{E}_2}^2$, can also be written as $\mathcal{E}_2(\bar{y}_2) = -N_2(h_2\bar{y}_2 + \frac{1}{2}J_2\bar{y}_2^2)$. Then the inverse temperature of bath is

$$\begin{aligned} \beta_2^* &= \frac{dS_2}{d\bar{y}_2}\left(\frac{d\mathcal{E}_2}{d\bar{y}_2}\right)^{-1} \\ &= \frac{1}{2(h_2 + J_2\bar{y}_2)} \ln\left(\frac{1+\bar{y}_2}{1-\bar{y}_2}\right). \end{aligned} \tag{18}$$

Note the limiting values for the bath temperature:

(i) For $\bar{y}_2 \to 1$, we have $\beta_2^* \to \infty$, which corresponds to bath temperature of zero degree Kelvin.

(ii) For $\bar{y}_2 \to 0$, $\beta_2^* \to 0$, or in other words, the bath is most disordered at arbitrarily high temperatures.

IV. EQUILIBRIUM PROPERTIES AND STABILITY

It is straightforward to calculate the free energy $A(y_1)$ from the partition function by the standard methods of Hubbard-Stratonovich transformation or the saddle point approximation. Thus we obtain

$$A(y_1) = \frac{1}{2} J_1 {y_1}^2 - \frac{1}{\beta_2^*} \ln\left[2\cosh\{\beta_2^*(h_1 + J_{12}\bar{y}_2 + J_1 y_1)\}\right]. \tag{19}$$

The stationarity condition $\partial A/\partial y_1 = 0$ yields a self-consistent equation for the equilibrium magnetisation per spin of system 1:

$$\bar{y}_1 = \tanh\left[\beta_2^*(h_1 + J_{12}\bar{y}_2 + J_1\bar{y}_1)\right]. \tag{20}$$

Usually, the analogue of this equation in the Curie-Weiss model is analysed for $h_1 = 0$ case to infer the existence of a critical temperature, above which the system is paramagnetic and below which it is ferromagnetic. In the ferromagnetic phase, two values of magnetisation $\pm|\bar{y}_1|$ are equally allowed, which actually reflects the symmetry of the hamiltonian.

In the present case, even in the absence of external field ($h_1 = 0$), there is an effective magnetic field $J_{12}\bar{y}_2$ due to long range interaction between system and the bath. Thus at high temperatures, we have a unique minimum of free energy at a non-zero value of magnetisation. Thus the sample is magnetised even at high temperatures. As the temperature is lowered, a metastable solution for magnetisation also appears alongwith the global equilibrium solution. The limit of metastability (defined by the inverse temperature $\beta_2^{(\mathrm{m})}$ at which the metastable state appears while lowering the temperature of the bath) can be calculated by finding the point of inflexion, where both first and second order derviatives of free energy vanish. The latter condition yields

$$\cosh\left[\beta_2^{(\mathrm{m})}(h_1 + J_{12}\bar{y}_2 + J_1\bar{y}_1)\right] = \sqrt{\beta_2^{(\mathrm{m})} J_1}. \tag{21}$$

Using the above condition alongwith Eq. (20), we can show that

$$\bar{y}_1 = \pm\sqrt{1 - \frac{1}{\beta_2^{(\mathrm{m})} J_1}} \tag{22}$$

From this equation, it is clear that $\beta_2^{(\mathrm{m})} J_1 \geq 1$. The condition, $\beta_2^{(\mathrm{m})} J_1 = 1$ implies that $\bar{y}_1 = 0$. But for $h_1 = 0$, this stationary solution is satisfied only for $J_{12} = 0$, (see Eq. (20) above). On the other hand, for $J_{12} \neq 0$, the stationary solution is non-zero. Thus we see that the condition (22) can be satisfied by $\bar{y}_1 \neq 0$ for an inverse temperture $\beta_2^{(\mathrm{m})}$ which implies that the bath temperature is lower than the critical temperature for the usual para-Ferro transition which obeys $\beta_2^{(\mathrm{crit})} J_1 = 1$. The actual temperature for limit of metastability may be calculated from Eqs. (20) and (22).

V. SUMMARY

We have introduced a new kind of ensemble to generalise the usual treatment of a thermal contact between system and heat bath by including long range interactions between them. The derivation is motivated by the standard derivation of the canonical ensemble from the microcanonical ensemble. However, the crucial difference is the lack of additivity of the energy. This does not yield exponential Boltzmann distributions. The form of the distributions is strongly dependent on the form of hamiltonian of the total sample plus bath system. Thus incorporating long range interactions makes the problem more involved as we have to specify a microscopic model for the bath as well as the nature of long range interactions between the system and the bath. In this paper, we have treated a very simple case when the interactions can be modelled by long range Ising model. An appropriate scaling of the interaction parameters with system or bath size helps to obtain a thermodynamic limit for the system properties. The observations for this analysis are that the usual para-ferro transition appears to be suppressed, with the presence of a net magnetisation for the system at high temperatures, even in the absence of an applied field. This happens because the long range interaction with the bath provides an effective magnetic field. Moreover, as the temperature is lowerd, there appears a metastable state. This happens at a temperature which is generally lower than the critical temperature of para-ferro transition in the Curie-Weiss model. It is hoped that the approach presented in this paper will motivate further studies with other model long-range interactions, such as slowly decaying interactions. This may facilitate the characterisation of thermodynamic behaviour in systems when interactions with the bath cannot be neglected.

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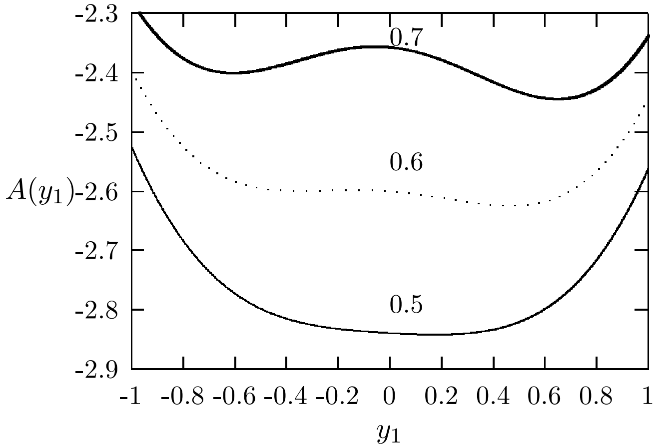

FIG. 1: Fig. 1: Free energy (Eq. (19)) plotted against system magnetisation for different bath temperatures, parameterised by the values of $\bar{y}_2$; increasing values imply decreasing bath temperature. The other paramters are set at $h_1 = 0, h_2 = 0.5, J_1 = 4.0, J_2 = 3.5, J_{12} = 0.05$.